

# Solving the Master Equation for Extremely Long Time Scale Calculations

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## Abstract

The dynamics of magnetic reversal process plays an important role in the design of the magnetic recording devices in the long time scale limit. In addition to long time scale, microscopic effects such as the entropic effect become important in magnetic nano-scale systems. Many advanced simulation methods have been developed, but few have the ability to simulate the long time scale limit and to accurately model the microscopic effects of nano-scale systems at the same time. We develop a new Monte Carlo method for calculating the dynamics of magnetic reversal at arbitrary long time. For example, actual calculations were performed up to  $10^{50}$  Monte Carlo steps. This method is based on microscopic interactions of many constituents and the master equation for magnetic probability distribution function is solved symbolically.

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## 1 Introduction

Studies on complex systems with meta-stable states are valuable in many disciplines. For instance, aging phenomena affect the properties of materials, magnetic relaxation processes determine the functions of magnetic recording media, and the study of first order phase transitions and spinodal decomposition have wide applications. Often, slow dynamics plays a central role in the understanding of these complex systems. When no analytic solutions are available, numerical simulations are the only tools to study these systems. In a Monte Carlo simulation, the meta-stable states could manifest as apparently stable or “equilibrium” states. Only after a very long time the simulation could

overcome the free energy barrier and go into equilibrium. When using the standard Metropolis algorithm, this time scale may become unattainable even with the fastest computer available. Hence advanced Monte Carlo techniques such as the Absorbing Markov Chains algorithm [1], which is a generalization of the N-fold way method [2], and the Projection Method [3] have been developed to address this issue. These methods have been used to study magnetic reversal [4,5,6]. In some cases, where the difficulties of meta-stability are not too serious, conventional Monte Carlo methods are also used [7,8,9,10].

In this paper, we will present a new method of calculating the dynamics of systems with meta-stable states by solving the master equation for magnetic probability distribution function symbolically. We illustrate our method in the context of magnetic reversal on the two dimensional Ising square lattice.

## 2 Method

The Ising model is a basic model to study the phase transition, and has also been used as a standard benchmark model for testing new algorithms [4,11,12,13,14,15,16,17,18,19,20]. The Hamiltonian for the Ising model is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i = E - hM \quad (1)$$

where  $s_i = \pm 1$ . The first summation is over nearest neighbors; the second summation is over all lattice sites.  $J$  and  $h$  are the exchange constant and external field respectively. We define two symbols  $E$  and  $M$  as the energy of the exchange part and the magnetization part,

$$\begin{aligned} E &= -J \sum_{\langle i,j \rangle} s_i s_j \\ M &= \sum_i s_i \end{aligned} \quad (2)$$

Ideally, to study the dynamics of magnetic reversal on the Ising model, the microscopic master equation,

$$\frac{dP(\sigma, t)}{dt} = \sum_{\sigma'} \omega(\sigma|\sigma') P(\sigma', t) - \omega(\sigma'|\sigma) P(\sigma, t) \quad (3)$$

is to be solved.  $\sigma$  denotes the microscopic state of the system,  $\omega(\sigma|\sigma')$  is the transition rate from  $\sigma'$  to  $\sigma$ , and  $P(\sigma, t)$  is the probability distribution of the state  $\sigma$  at time  $t$ . For a lattice with  $N$  sites, Eq. (3) is a set of  $2^N$  coupled

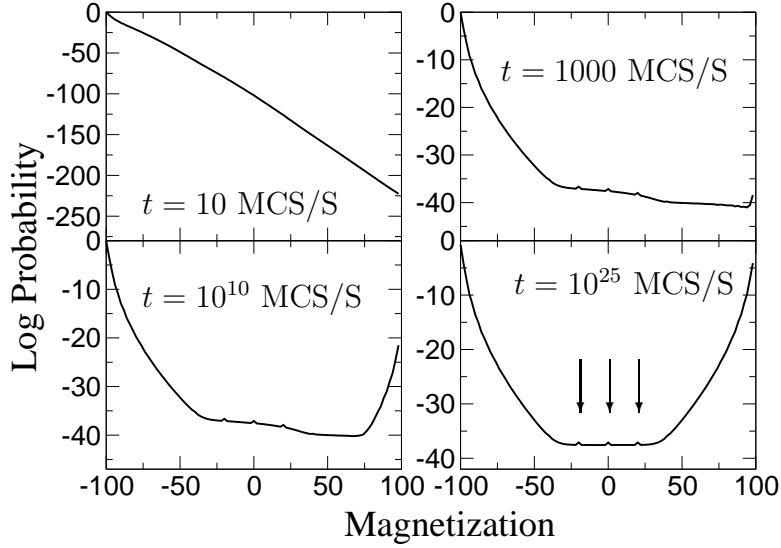


Fig. 1. Log of probability distributions plotted at  $t = 10, 1000, 10^{10}$  and  $10^{25}$  for  $L = 10, T = 0.44T_c$  and  $h = 0$ . Initial condition is  $P(t = 0, M) = \delta_{M, -100}$ . At time  $t = 10^{25}$ , the probability distribution is almost indistinguishable from the equilibrium distribution. The little spikes marked with arrows are due to band structure of the Ising model (Fig. 2). Equilibrium probability distribution was generated using the Wang-Landau method up to correction factor of  $\log(f) = 1.25 \times 10^{-8}$ . Error bars are smaller than the thickness of the lines.

differential equations and solving them is infeasible. Instead the dynamics can be approximated by writing the master equation in terms of the total magnetization  $M$ ,

$$\frac{dP(M, t)}{dt} = \sum_{M'} \omega(M|M')P(M', t) - \omega(M'|M)P(M, t) \quad (4)$$

which is a set of  $N + 1$  differential equations. The approximate form of the macroscopic transition rates  $\omega(M|M')$  was discussed by Lee *et.al.* [21]. We made identical approximations in the transition rates as the “mean field dynamics 2” (MFD2) obtained by Lee *et.al.* [21]. Other ways of obtaining the transition rates, such as the Transition Matrix Monte Carlo method [22], may also be used. Our main contribution in this paper is in the way of solving the macroscopic master equation (Eq. (4)). Our results are accurate to within the validity of basic approximations in the transition rates. However, the gain in efficiencies and accuracies of our results are many orders of magnitude larger than most Monte Carlo methods.

As in Ref. [21] the equilibrium distribution is used to calculate the transition rates. With this approximation, not all microscopic information is available. The region of validity for this approximation will be discussed later.

An efficient Monte Carlo algorithm to calculate the density of states has been recently proposed by Wang and Landau [19,20]. We have used the Wang-Landau [19,20] algorithm to estimate the density of states as a function of exchange energy and magnetization  $g(E, M)$ , with  $E$  and  $M$  defined by Eq. (2). For a given  $\beta = 1/k_B T$  and  $h$ , the joint probability distribution  $P_{\beta,h}^{eq}(E, M)$  is then obtained using Boltzmann weights as

$$P_{\beta,h}^{eq}(E, M) = g(E, M) \exp(-\beta[E - hM]) / \mathcal{Z}(\beta, h) \quad (5)$$

$\mathcal{Z}$  is the partition function given by,

$$\mathcal{Z}(\beta, h) = \sum_{E,M} g(E, M) \exp(-\beta[E - hM]) \quad (6)$$

Finally, the equilibrium probability distribution of  $M$  can be obtained,

$$P_{\beta,h}^{eq}(M) = \sum_E P_{\beta,h}^{eq}(E, M) \quad (7)$$

For a lattice with  $L^2 = N$  sites, there are  $N + 1$  possible values of magnetization. Then the master equation (Eq. (4)) can be written in a matrix form,

$$\frac{d\vec{P}(t)}{dt} = \mathcal{A} \cdot \vec{P}(t) \quad (8)$$

where the  $(N + 1)$  dimensional vector  $\vec{P}(t)$  is

$$\vec{P}(t) = \begin{pmatrix} P(M = -N, t) \\ \vdots \\ P(M = 0, t) \\ \vdots \\ P(M = +N, t) \end{pmatrix} \quad (9)$$

In this paper, we present a way to calculate the explicit solution to Eq. (8). We restrict the transitions to  $|\Delta M| = 2$ . This is a vital component of our work and we shall elaborate its implications and the conditions in which it is valid. Transitions which involve  $|\Delta M| = 2$  are all single spin flip moves or any move which flip  $N$  spins from  $+1$  to  $-1$  and  $N + 1$  spins from  $-1$  to  $+1$  (or vice versa). At low temperature and low field, we do not expect to observe many cluster flips or multiple spin flip transitions. Hence our assumption is valid at low temperature and low field. Incidentally, the process of magnetic reversal at

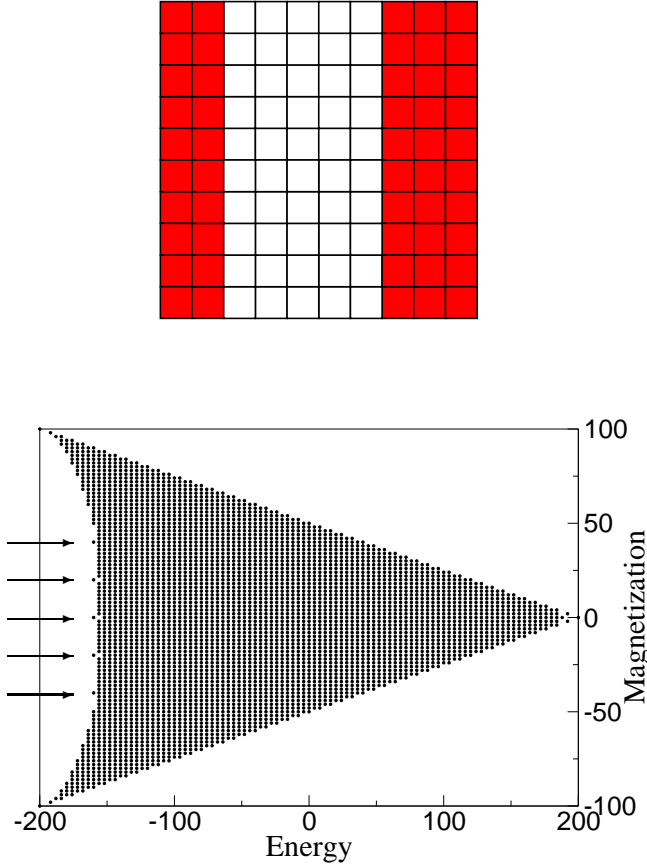


Fig. 2. The upper figure shows a band structure that is the origin of spikes observed in the probability distribution of Fig. 1. These are local energy minimum configurations, and any single spin flip increases the energy. The lower figure shows the domain of accessible state for  $L = 10$  Ising model. The minimum energy state with  $M = 0$  is  $E = -160$  or  $E = E_g + 4L$ , where  $E_g$  is the ground state energy. Arrows indicate band structure states shown in the upper figure, and their exact density of states can also be trivially calculated.

low temperature and field is via the single-droplet process [23,24,25,26]. This is also the domain where the approximation to our transition rates is valid. At high temperatures, other magnetic reversal processes such as the multi-droplet process dominate and our approximation becomes not accurate in this regime. Short time scale behavior becomes important at high temperatures and other Monte Carlo methods may be used.

With the constraint  $|\Delta M| = 2$ , the transition rate  $\omega$  is written as

$$\omega(M_j|M_i) \approx \begin{cases} P^{eq}(M_j)/[P^{eq}(M_j) + P^{eq}(M_i)] & |i - j| \leq 1 \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

if the Glauber rate is employed. The Metropolis rate can also be used, and we compare the results obtained by both rates in Table 1.

For the transition rates given by Eq. (10), the master equation (Eq. (8)) can be reduced into one linear differential equation with constant coefficients and the analytic solutions for this equation is known [27]. A procedure to derive the solution is given in an appendix. The general solution is of the form,

$$\vec{P}(t) = \sum_{i=0}^N \alpha_i \vec{v}_i \exp(\lambda_i t) \quad (11)$$

where  $\lambda_i$  and  $\vec{v}_i$  are the eigenvalues and eigenvectors of the matrix  $\mathcal{A}$  and  $\alpha_i$  are constant coefficients determined by solving Eq. (11) with initial conditions,

$$\vec{P}(0) = \sum_{i=0}^N \alpha_i \vec{v}_i \quad (12)$$

We used MATHEMATICA to calculate  $\alpha_i$ ,  $\vec{v}_i$  and  $\lambda_i$  numerically, and  $\vec{P}(t)$  is represented symbolically as a function of time. We have also made use of a MATHEMATICA function for setting arbitrary precisions and compared our results for calculations with different precisions. With  $\vec{P}(t)$  evaluated symbolically, other magnetic quantities, such as  $M(t)$ , can be evaluated symbolically as well.

The initial conditions were set with all the spins in the  $-1$  position and the external field always favors spin configurations with  $s_i = +1$ . Our simulations were performed on a dual 2 GHz PowerMac G5 PC, with over 95% of the computing resources devoted to calculating the equilibrium density of states using the Wang-Landau method [19,20].

### 3 Results

All eigenvalues are real and negative except for the largest eigenvalue which is zero. The probability distribution can be re-written as,

$$\vec{P}(t) = \alpha_0 \vec{v}_0 + \sum_{i=1}^N \alpha_i \vec{v}_i \exp(-|\lambda_i|t) \quad (13)$$

$$= \vec{P}^{eq} + \sum_{i=1}^N \alpha_i \vec{v}_i \exp(-|\lambda_i|t) \quad (14)$$

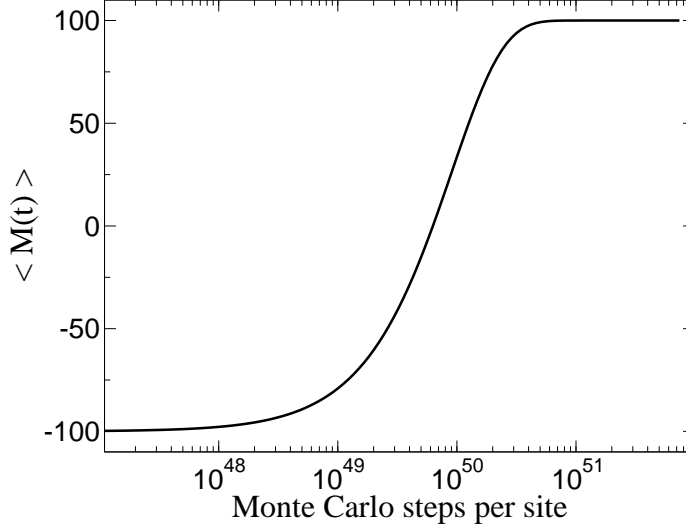


Fig. 3. Magnetization versus time curve for  $L = 10, T = 0.11T_c, h/J = 0.25$ . Equilibrium probability distribution was estimated using the Wang-Landau method up to a correction factor  $\log(f) = 1.25 \times 10^{-8}$ . In agreement with previous works [25,26], the switching duration is approximately equal to the lifetime. Error bars are much smaller than thickness of the line.

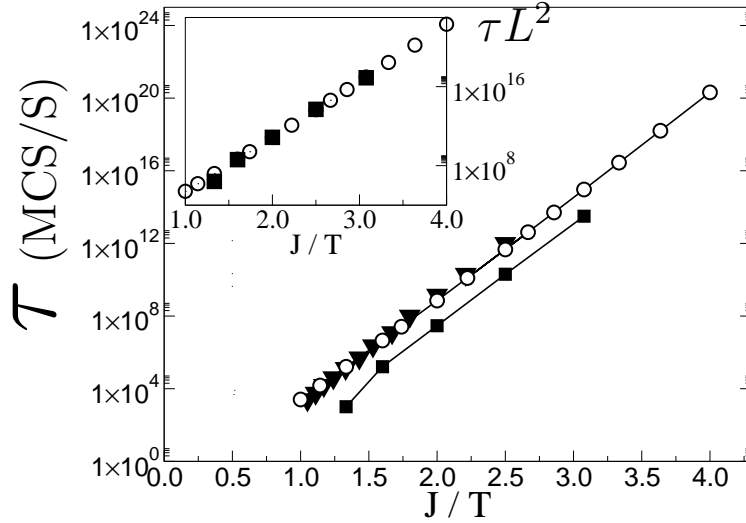


Fig. 4. Plot of switching time  $\tau$  at  $h/J = 0.75$ , which shows very good agreement with previous studies by Novotny [4]. Lattice sizes are  $L = 10$  (circles) and  $L = 50$  (squares). Triangles show the results reported by Novotny [4] for  $L = 10$  lattice.

where  $\alpha_0$  and  $\vec{v}_0$  are the coefficients and eigenvector corresponding to the largest eigenvalue (which is zero), and  $\alpha_0 \vec{v}_0 = \vec{P}^{eq}$ . Hence,

$$\lim_{t \rightarrow \infty} \vec{P}(t) = \vec{P}^{eq} \quad (15)$$

Fig. 1 shows the time evolution of the probability distribution function for  $L = 10$ ,  $T = 0.44T_c$  and  $h = 0$ . The magnetization was set to  $-N$  at  $t = 0$  and allowed to evolve via the master equation. At  $t = 10$ , probability distribution falls off exponentially from near 1 at  $M = -100$  to  $\exp(-225)$  at  $M = 100$ . At  $t = 10^{10}$ , the probability distribution at  $M = 100$  increases and we begin to see two peaks, but the peak at  $M = 100$  is 20 orders of magnitude smaller. At  $t = 10^{25}$ , the probability distribution is almost symmetric and indistinguishable from the equilibrium probability distribution. Spikes indicated with arrows originate from special band structures of the Ising model (Fig. 2). These band structures are local energy minimums, any single spin flip from these structures resulted in an increase of energy. Fig. 2 also shows the domain of accessible states for  $L = 10$ , and arrows indicate band structures states. They have equal spacing in magnetization of  $\Delta M = 2L$  and their energies are  $E_g + 4L$ , where  $E_g$  is the ground state energy. We have demonstrated our calculation of the probability distribution with zero external field, because the spikes in the probability distribution appear most prominently with  $h = 0$ .

We are also interested in studying magnetic switching in an external field where a direct comparison with previous work is available. Fig. 3 shows reversal of magnetization in an external field at  $T = 0.11T_c$  and  $h/J = 0.25$  for  $L = 10$  lattice. In agreement with previous works [25,26] the average switching duration is approximately equal to the lifetime.

The temperature dependence of the switching time can be studied by plotting the switching times versus the inverse temperature at  $h/J = 0.75$  (Fig. 4). Here we define the switching time as the time when the average magnetization reaches zero ( $\langle M(t) \rangle = 0$ ). The data for  $L = 10$  are compared with those by Novotny [4]. We obtained very good agreement with previous works. In the insert of Fig. 4, we plot the switching time  $\times$  system size as a function of the inverse temperature. The data for  $L = 10$  and  $L = 50$  collapse into a single curve, as expected in the single-droplet regime. In contrast with the other method employed in Ref. [3] where  $\tau$  is calculated directly, the present method calculates the entire probability distribution of the master equation that allows us to calculate other quantities such as average magnetization.

There are two sources of approximation in our method; the first one is the approximation of transition rates using equilibrium distribution, the second one originated from uncertainty in the density of states estimated from Wang-Landau method. The effects of uncertainties on a  $L = 10$  lattice in a field of  $h/J = 0.75$  are summarized in Table 1. In the Wang-Landau algorithm, the correction factor  $f$  is used in the process of refining the density of states. The final value of  $f$  is related to the accuracy of the calculation, and smaller “ $\log(f)$ ” values corresponds to more accurate equilibrium distributions. Our results suggest that running the Wang-Landau algorithm to  $\log(f)$  value of  $1.25 \times 10^{-6}$  is sufficient to within our simulation precision. Table 1 also shows



$J/T$	Rates	$\log(f)$ values	$\tau$ (MCS/S)	$\Delta\tau$
2.67	Glauber	$1.70 \times 10^{-4}$	$4.1 \times 10^{12}$	$5.8 \times 10^{11}$
2.67	Glauber	$1.25 \times 10^{-6}$	$4.1 \times 10^{12}$	$3.9 \times 10^{10}$
2.67	Glauber	$1.25 \times 10^{-8}$	$4.1 \times 10^{12}$	$2.8 \times 10^{10}$
2.67	Metropolis	$1.70 \times 10^{-4}$	$3.9 \times 10^{12}$	$5.6 \times 10^{11}$
2.67	Metropolis	$1.25 \times 10^{-6}$	$4.0 \times 10^{12}$	$3.7 \times 10^{10}$
2.67	Metropolis	$1.25 \times 10^{-8}$	$4.0 \times 10^{12}$	$2.7 \times 10^{10}$
1.00	Glauber	$1.70 \times 10^{-4}$	2538	304
1.00	Glauber	$1.25 \times 10^{-6}$	2550	21
1.00	Glauber	$1.25 \times 10^{-8}$	2556	13
1.00	Metropolis	$1.70 \times 10^{-4}$	1524	182
1.00	Metropolis	$1.25 \times 10^{-6}$	1527	12
1.00	Metropolis	$1.25 \times 10^{-8}$	1531	7.8

Table 1

Comparing results using Glauber and Metropolis transition rates and using different estimates of equilibrium distributions. “ $\log(f)$  values” given in the third column are the values of correction factors in Wang-Landau method [19] on  $L = 10$  lattice with  $h/J = 0.75$ .

the dependence of switching time  $\tau$  with Glauber and Metropolis rates. The Metropolis rates are given by,

$$\omega(M|M') \approx \min \left[ 1, \frac{P^{eq}(M)}{P^{eq}(M')} \right] \text{ for } |i - j| \leq 1 \quad (16)$$

There is no significant difference in the switching time between Glauber and Metropolis transition rates for low temperature ( $J/T = 2.67$ ). But they differ at high temperature because the approximation to the transition rates becomes less accurate at high temperatures. The uncertainties in the switching time,  $\Delta\tau$  was obtained from several independent runs.

## 4 Conclusion

In conclusion, we derived an explicit expression for the magnetic probability distribution as a function of time. With the probability distribution, all dynamical information is available. And we used the information to obtain consistent results with previous works. Another advantage is that dynami-

cal properties can be evaluated to arbitrary long time without requiring more computational resources. Lastly, we should mention that our method is general and not restricted to discrete systems or any specific models. Future development of the present method should focus on calculation of larger lattice sizes. Currently, lattice sizes are limited by the efficiency of Wang-Landau algorithm to calculate joint density of states.

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## Appendix : Solutions to the Master Equation

A general procedure to solve the master equation will be presented in this appendix. Firstly, we shall introduce the mathematical notation, the probability distribution function  $P(M, t)$  will be denoted in a form of a vector,

$$\begin{pmatrix} P(M = -N, & t) \\ P(M = -N + 2, t) \\ \vdots \\ P(M = +N & , t) \end{pmatrix} = \begin{pmatrix} P_1(t) \\ P_2(t) \\ \vdots \\ P_{N+1}(t) \end{pmatrix} \quad (17)$$

Note that for an Ising model with  $N$  sites, with  $N$  being an even number, the number of possible magnetizations is  $N + 1$  with  $M = \{-N, \dots, 0, \dots, N\}$ . The master equation can be written in a matrix form,

$$\frac{d\vec{P}(t)}{dt} = \mathcal{A} \cdot \vec{P}(t) \quad (18)$$

where  $\mathcal{A}$  is a  $(N + 1) \times (N + 1)$  tridiagonal matrix with constant matrix elements. Suppose  $\mathcal{S}^{-1}\mathcal{A}\mathcal{S} = \mathcal{D}$ , where  $\mathcal{S}$  is a similarity transform and  $\mathcal{D}$  is a diagonal matrix. Then we have

$$\frac{d\vec{P}(t)}{dt} = \mathcal{S}\mathcal{D}\mathcal{S}^{-1} \cdot \vec{P}(t) \quad (19)$$

Defining a new vector  $\vec{Q}(t) = \mathcal{S}^{-1}\vec{P}(t)$ , we obtain

$$\frac{d\vec{Q}(t)}{dt} = \mathcal{D} \cdot \vec{Q}(t) \quad (20)$$

Since  $\mathcal{D}$  is a diagonal matrix, Eq. (20) is easily solved with  $Q_i(t) = C_i \exp(\lambda_i t)$ , where  $\lambda_i$  is the  $i$ th eigenvalue of  $\mathcal{A}$ . With  $\vec{P}(t) = \mathcal{S}\vec{Q}(t)$ , we have

$$\vec{P}(t) = \sum_i \alpha_i \vec{v}_i \exp(\lambda_i t) \quad (21)$$

We write  $\vec{P}$  in terms of the eigenvectors so that the constant coefficients  $\alpha_i$  can be easily found by initial conditions,

$$\vec{P}(t=0) = \sum_i \alpha_i \vec{v}_i \quad (22)$$

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